



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:50 AM GMT

PDB ID : 2IX3
Title : STRUCTURE OF YEAST ELONGATION FACTOR 3
Authors : Andersen, C.B.F.; Becker, T.; Blau, M.; Anand, M.; Halic, M.; Balar, B.; Mielke, T.; Boesen, T.; Pedersen, J.S.; Spahn, C.M.T.; Kinzy, T.G.; Andersen, G.R.; Beckmann, R.
Deposited on : 2006-07-06
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

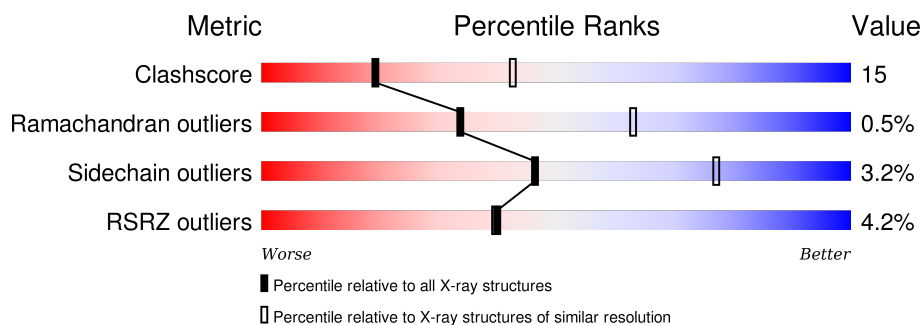
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	986	<div> <div>3%</div> <div>73%</div> <div>24%</div> <div>..</div> </div>
1	B	986	<div> <div>5%</div> <div>66%</div> <div>32%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	2976	-	-	-	X
2	SO4	A	2978	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	2974	-	X	X	X
2	SO4	B	2975	-	X	-	X

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 15213 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ELONGATION FACTOR 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	973	Total	C	N	O	S	0	0	1
			7579	4790	1297	1455	37			
1	B	973	Total	C	N	O	S	0	0	1
			7579	4790	1297	1455	37			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

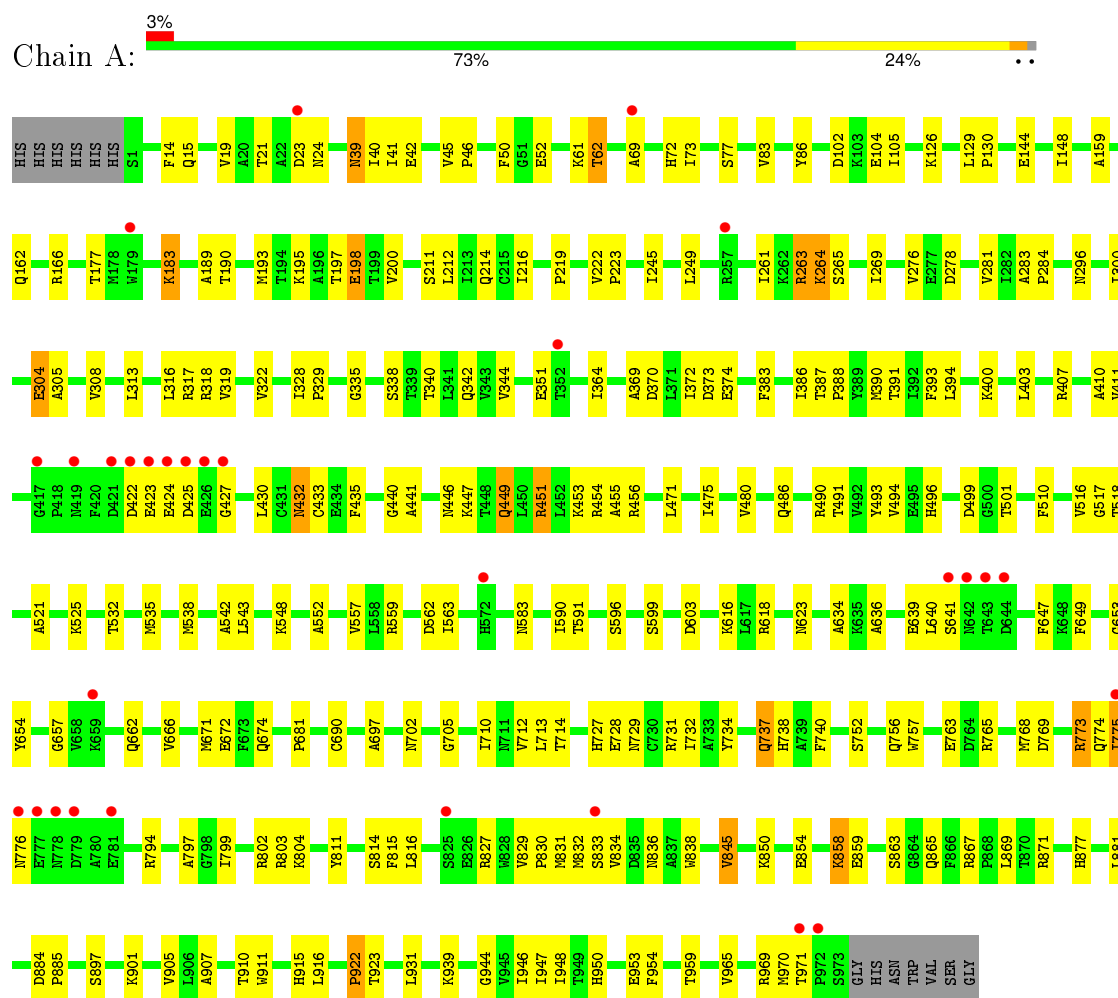
Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

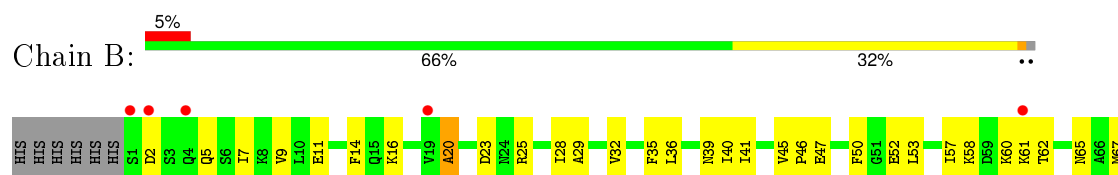
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: ELONGATION FACTOR 3



• Molecule 1: ELONGATION FACTOR 3



G943	G944	I948	T949	K956	N957	L958	T959	R969	M970	S973	GLY	HIS	ASN	TRP	VAL	SER	GLY	P830	M831	N836	E846	K850	M851	H852	E854	V855	E859	L869	K872	E875	E876	H877	C878	S879	K880	L881	D884	L887	S891	R892	L893	R894	G898	V902	A907	W911	H915	L916	E921	N924	R928	K936	K939	E940	F941	E942	R731	Y734	I735	E736	K737	H738	L747	T750	E753	Y754	W757	R758	D764	R765	E766	D769	R770	A771	N772	R773	Q774	I775	N776	E777	N778	D779	A780	E781	A782	M783	N784	K785	I786	F787	R794	A797	G798	I799	K804	F805	K806	Y811	S814	F815	L816	R827	A634	E635	A636	Y637	E638	E639	L640	S641	N642	D643	D644	L645	E646	F647	P652	G653	Y654	Q662	V666	M671	B672	F673	Q674	Y675	F676	G677	K680	P681	T684	D685	C690	R695	I696	A697	M702	G703	T708	L709	Y710	N711	V712	E716	L717	L718	K719	P719	E728	N729	C730	V492	Y493	V494	E495	H496	D499	G500	T501	D504	L508	B509	F510	K525	T532	M535	I536	A537	P538	P539	A542	R555	B559	T563	E568	P569	T570	N571	H572	L573	L581	D603	Y608	N611	Y612	B613	K616	L617	K618	K619	Y620	K621	G622	N623	E374	R375	I386	T387	P388	Y389	M390	F392	F393	L394	K397	D404	R407	A410	N413	V416	G417	P418	N419	D421	D422	E423	E424	E425	E426	G427	E428	C431	N432	G440	A441	N446	K447	R451	L452	K453	R454	A455	R456	R457	Y458	P463	C466	T491	D278	P279	Q280	V281	I282	A283	P284	F285	L290	P291	F297	N296	A298	T299	I300	A301	D302	A305	R306	E307	V308	T309	L310	L313	R317	R318	V319	G320	N321	V322	G323	E324	D325	E330	L331	S332	H333	Q342	K358	I359	V360	Y361	E362	Y363	I364	I367	D370	L371	D373	D278	P279	Q280	V281	I282	A283	P284	F285	L290	P291	F297	N296	A298	T299	I300	A301	D302	A305	R306	E307	V308	T309	L310	L313	R317	R318	V319	G320	N321	V322	G323	E324	D325	E330	L331	S332	H333	Q342	K358	I359	V360	Y361	E362	Y363	I364	I367	D370	L371	D373	T181	K182	K183	E184	V185	K186	M193	T194	K195	A196	T197	E198	T199	V200	N202	K203	D204	I205	E206	R207	P219	V222	P223	V226	A231	V238	T239	P240	A124	I125	K126	L129	P130	E256	R257	E258	I261	K262	R263	K264	S265	A266	V267	I268	I269	N272	C273	K274	L275	I372	E277	K101	D102	K103	E104	I105	A109	T112	L113	I116	V117	N121	P122	V123	A124	I125	K126	L129	P130	E256	R257	E258	I261	K262	R263	K264	S265	A266	V267	I268	I269	N272	C273	K274	L275	I372	E277	K135	I136	T139	N140	K145	T148	R166	M167	P168	E169	P172	D180	K182	K183	E184	V185	K186	M193	T194	K195	A196	T197	E198	T199	V200	N202	K203	D204	I205	E206	R207	P219	V222	P223	V226	A231	V238	T239	P240	A124	I125	K126	L129	P130	E256	R257	E258	I261	K262	R263	K264	S265	A266	V267	I268	I269	N272	C273	K274	L275	I372	E277	K101	D102	K103	E104	I105	A109	T112	L113	I116	V117	N121	P122	V123	A124	I125	K126	L129	P130	E256	R257	E258	I261	K262	R263	K264	S265	A266	V267	I268	I269	N272	C273	K274	L275	I372	E277	K135	I136	T139	N140	K145	T148	R166	M167	P168	E169	P172	D180	K182	K183	E184	V185	K186	M193	T194	K195	A196	T197	E198	T199	V200	N202	K203	D204	I205	E206	R207	P219	V222	P223	V226	A231	V238	T239	P240	A124	I125	K126	L129	P130	E256	R257	E258	I261	K262	R263	K264	S265	A266	V267	I268	I269	N272	C273	K274	L275	I372	E277	K101	D102	K103	E104	I105	A109	T112	L113	I116	V117	N121	P122	V123	A124	I125	K126	L129	P130	E256	R257	E258	I261	K262	R263	K264	S265	A266	V267	I268	I269	N272	C273	K274	L275	I372	E277	K135	I136	T139	N140	K145	T148	R166	M167	P168	E169	P172	D180	K182	K183	E184	V185	K186	M193	T194	K195	A196	T197	E198	T199	V200	N202	K203	D204	I205	E206	R207	P219	V222	P223	V226	A231	V238	T239	P240	A124	I125	K126	L129	P130	E256	R257	E258	I261	K262	R263	K264	S265	A266	V267	I268	I269	N272	C273	K274	L275	I372	E277	K101	D102	K103	E104	I105	A109	T112	L113	I116	V117	N121	P122	V123	A124	I125	K126	L129	P130	E256	R257	E258	I261	K262	R263	K264	S265	A266	V267	I268	I269	N272	C273	K274	L275	I372	E277	K135	I136	T139	N140	K145	T148	R166	M167	P168	E169	P172	D180	K182	K183	E184	V185	K186	M193	T194	K195	A196	T197	E198	T199	V200	N202	K203	D204	I205	E206	R207	P219	V222	P223	V226	A231	V238	T239	P240	A124	I125	K126	L129	P130	E256	R257	E258	I261	K262	R263	K264	S265	A266	V267	I268	I269	N272	C273	K274	L275	I372	E277	K101	D102	K103	E104	I105	A109	T112	L113	I116	V117	N121	P122	V123	A124	I125	K126	L129	P130	E256	R257	E258	I261	K262	R263	K264	S265	A266	V267	I268	I269	N272	C273	K274	L275	I372	E277	K135	I136	T139	N140	K145	T148	R166	M167	P168	E169	P172	D180	K182	K183	E184	V185	K186	M193	T194	K195	A196	T197	E198	T199	V200	N202	K203	D204	I205	E206	R207	P219	V222	P223	V226	A231	V238	T239	P240	A124	I125	K126	L129	P130	E256	R257	E258	I261	K262	R263	K264	S265	A266	V267	I268	I269	N272	C273	K274	L275	I372	E277	K101	D102	K103	E104	I105	A109	T112	L113	I116	V117	N121	P122	V123	A124	I125	K126	L129	P130	E256	R257	E258	I261	K262	R263	K264	S265	A266	V267	I268	I269	N272	C273	K274	L275	I372	E277	K135	I136	T139	N140	K145	T148	R166	M167	P168	E169	P172	D180	K182	K183	E184	V185	K186	M193	T194	K195	A196	T197	E198	T199	V200	N202	K203	D204	I205	E206	R207	P219	V222	P223	V226	A231	V238	T239	P240	A124	I125	K126	L129	P130	E256	R257	E258	I261	K262	R263	K264	S265	A266	V267	I268	I269	N272	C273	K274	L275	I372	E277	K101	D102	K103	E104	I105	A109	T112	L113	I116	V117	N121	P122	V123	A124	I125	K126	L129	P130	E256	R257	E258	I261	K262	R263	K264	S265	A266	V267	I268	I269	N272	C273	K274	L275	I372	E277	K135	I136	T139	N140	K145	T148	R166	M167	P168	E169	P172	D180	K182	K183	E184	V185	K186	M193	T194	K195	A196	T197	E198	T199	V200	N202	K203	D204	I205	E206	R207	P219	V222	P223	V226	A231	V238	T239	P240	A124	I125	K126	L129	P130	E256	R257	E258	I261	K262	R263	K264	S265	A266	V267	I268	I269	N272	C273	K274	L275	I372	E277	K101	D102	K103	E104	I105	A109	T112	L113	I116	V117	N121	P122	V123	A124	I125	K126	L129	P130	E256	R257	E258	I261	K262	R263	K264	S265	A266	V267	I268	I269	N272	C273	K274	L275	I372	E277	K135	I136	T139	N140	K145	T148	R166	M167	P168	E169	P172	D180	K182	K183	E184	V185	K186	M193	T194	K195	A196	T197	E198	T199	V200	N202	K203	D204	I205	E206	R207	P219	V222	P223	V226	A231	V238	T239	P240	A124	I125	K126	L129	P130	E256	R257	E258	I261	K262	R263	K264	S265	A266	V267	I268	I269	N272	C273	K274	L275	I372	E277	K101	D102	K103	E104	I105	A109	T112	L113	I116	V117	N121	P122	V123	A124	I125	K126	L129	P130	E256	R257	E258	I261	K262	R263	K264	S265	A266	V267	I268	I269	N272	C273	K274	L275	I372	E277	K135	I136	T139	N140	K145	T148	R166	M167	P168	E169	P172	D180	K182	K183	E184	V185	K186	M193	T194	K195	A196	T197	E198	T199	V200	N202	K203	D204	I205	E206	R207	P219	V222	P223	V226	A231	V238	T239	P240	A124	I125	K126	L129	P130	E256	R257	E258	I261	K262	R263	K264	S265	A266	V267	I268	I269	N272	C273	K274	L275	I372	E277	K101	D102	K103	E104	I105	A109	T112	L113	I116	V117	N121	P122	V123	A124	I125	K126	L129	P130	E256	R257	E258	I261	K262	R263	K264	S265	A266	V267	I268	I269	N272	C273	K274	L275	I372	E277	K135	I136	T139	N140	K145	T148	R166	M167	P168	E169	P172	D180	K182	K183	E184	V185	K186	M193	T194	K195	A196	T197	E198	T199	V200	N202	K203	D204	I205	E206	R207	P219	V222	P223	V226	A231	V238	T239	P240	A124	I125	K126	L129	P130	E256	R257	E258	I261	K262	R263	K264	S265	A266	V267	I268	I269	N272	C273	K274	L275	I372	E277	K101	D102	K103	E104	I105	A109	T112	L113	I116	V117	N121	P122	V123	A124	I125	K126	L129	P130	E256	R257	E258	I261	K262	R263	K264	S265	A266	V267	I268	I269	N272	C273	K274	L275	I372	E277	K135	I136	T139	N140	K145	T148	R166	M167	P168	E169	P172	D180	K182	K183	E184	V185	K186	M193	T194	K195	A196	T197	E198	T199	V200	N202	K203	D204	I205	E206	R207	P219	V222	P223	V226	A231	V238	T239	P240	A124	I125	K126	L129	P130	E256	R257	E258	I261	K262	R263	K264	S265	A266	V267	I268	I269	N272	C273	K274	L275	I372	E277	K101	D102	K103	E104	I105	A109	T112	L113	I116	V117	N121	P122	V123	A124	I125	K126	L129	P130	E256	R257	E258	I261	K262	R263	K264	S265	A266	V267	I268	I269	N272	C273	K274	L275	I372	E277	K135	I136	T139	N140	K145	T148	R166	M167	P168	E169	P172	D180	K182	K183	E184	V185	K186	M193	T194	K195	A196	T197	E198	T199	V200	N202	K203	D204	I205	E206	R207	P219	V222	P22
------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.61Å 110.66Å 212.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.63 – 2.70 20.16 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.63-2.70) 100.0 (20.16-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.09 (at 2.71Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.216 , 0.269 0.215 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	48.9	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 63818 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15213	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.41	0/7717	0.62	0/10456
1	B	0.39	0/7717	0.60	0/10456
All	All	0.40	0/15434	0.61	0/20912

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7579	0	7627	215	0
1	B	7579	0	7627	249	0
2	A	30	0	0	3	0
2	B	25	0	0	3	0
All	All	15213	0	15254	460	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (460) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:769:ASP:HB2	1:B:774:GLN:NE2	1.55	1.22
1:B:774:GLN:O	1:B:776:ASN:N	1.98	0.96
1:A:731:ARG:H	1:A:915:HIS:HD2	1.13	0.96
1:B:262:LYS:HE3	1:B:296:ASN:ND2	1.83	0.92
1:B:372:ILE:HD11	1:B:410:ALA:HB1	1.51	0.91
1:A:183:LYS:HD3	1:A:183:LYS:H	1.36	0.90
1:A:318:ARG:CZ	1:A:423:GLU:HG3	2.01	0.89
1:A:773:ARG:O	1:A:774:GLN:HG2	1.74	0.87
1:B:731:ARG:H	1:B:915:HIS:HD2	1.22	0.85
1:B:50:PHE:HZ	1:B:83:VAL:HG13	1.40	0.85
1:B:67:MET:CE	1:B:94:ILE:HG23	2.07	0.84
1:A:794:ARG:HD3	1:A:831:MET:HE1	1.61	0.83
1:B:769:ASP:CB	1:B:774:GLN:NE2	2.39	0.83
1:A:881:LEU:HD13	1:A:907:ALA:HA	1.61	0.82
1:B:671:MET:SD	1:B:712:VAL:HG11	2.21	0.81
1:A:525:LYS:HE2	1:A:557:VAL:HG11	1.64	0.80
1:A:21:THR:HG23	1:A:23:ASP:H	1.46	0.80
1:A:45:VAL:HG11	1:A:86:TYR:CZ	2.19	0.78
1:A:671:MET:HG2	1:A:672:GLU:N	1.97	0.78
1:B:794:ARG:HD3	1:B:831:MET:HE3	1.65	0.78
1:B:769:ASP:HB2	1:B:774:GLN:HE21	1.44	0.77
1:A:532:THR:HG23	1:A:535:MET:H	1.50	0.77
1:B:263:ARG:NH2	1:B:264:LYS:HE3	2.00	0.77
1:B:14:PHE:CE2	1:B:52:GLU:HB3	2.21	0.76
1:B:67:MET:HE3	1:B:94:ILE:HG23	1.65	0.76
1:A:729:ASN:HD22	1:A:865:GLN:HG3	1.51	0.75
1:A:697:ALA:HB2	1:A:959:THR:HG21	1.68	0.75
1:B:769:ASP:CB	1:B:774:GLN:HE21	1.98	0.75
1:B:197:THR:HG22	1:B:245:ILE:HD13	1.67	0.74
1:B:731:ARG:H	1:B:915:HIS:CD2	2.04	0.73
1:A:647:PHE:HB2	1:A:881:LEU:HA	1.69	0.73
1:B:50:PHE:CZ	1:B:83:VAL:HG13	2.24	0.72
1:A:671:MET:SD	1:A:712:VAL:HG11	2.30	0.72
1:B:262:LYS:HE3	1:B:296:ASN:HD21	1.53	0.72
1:B:67:MET:CE	1:B:109:ALA:HA	2.20	0.72
1:B:265:SER:O	1:B:269:ILE:HG13	1.91	0.71
1:B:279:PRO:HG3	1:B:418:PRO:HG2	1.73	0.71
1:B:72:HIS:CE1	1:B:773:ARG:HD2	2.25	0.70
1:A:731:ARG:HH12	1:A:865:GLN:NE2	1.88	0.70
1:A:697:ALA:HB2	1:A:959:THR:CG2	2.22	0.70
1:B:183:LYS:H	1:B:183:LYS:HD3	1.57	0.70
1:B:772:ASN:HB3	1:B:846:GLU:HG3	1.73	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:MET:HE2	1:B:109:ALA:HA	1.74	0.69
1:B:718:LEU:HD12	1:B:719:PRO:HD2	1.75	0.68
1:B:815:PHE:HB2	1:B:831:MET:CE	2.24	0.68
1:A:969:ARG:HH11	1:A:969:ARG:HG3	1.57	0.68
1:B:718:LEU:HD11	1:B:806:LYS:HD2	1.77	0.67
1:B:532:THR:CG2	1:B:535:MET:HG3	2.24	0.67
1:B:263:ARG:HH22	1:B:264:LYS:HE3	1.59	0.67
1:A:881:LEU:HD13	1:A:907:ALA:CA	2.25	0.67
1:A:276:VAL:HB	1:A:319:VAL:HG11	1.78	0.66
1:B:850:LYS:O	1:B:854:GLU:HG3	1.95	0.66
1:B:799:ILE:HG22	1:B:855:VAL:HG21	1.78	0.66
1:B:757:TRP:CH2	1:B:765:ARG:HD2	2.29	0.66
1:A:532:THR:HG22	1:A:535:MET:HG3	1.78	0.66
1:A:649:PHE:CD1	1:A:910:THR:HG21	2.31	0.66
1:A:41:ILE:HD12	1:A:46:PRO:HD3	1.75	0.66
1:A:518:THR:HG21	2:B:2977:SO4:O3	1.95	0.66
1:A:144:GLU:O	1:A:148:ILE:HG13	1.96	0.66
1:B:634:ALA:HB1	1:B:637:TYR:CE2	2.31	0.66
1:B:647:PHE:HB2	1:B:881:LEU:HA	1.78	0.65
1:A:731:ARG:H	1:A:915:HIS:CD2	2.05	0.65
1:A:40:ILE:HG13	1:A:41:ILE:HG13	1.78	0.65
1:A:731:ARG:N	1:A:915:HIS:HD2	1.92	0.65
1:A:666:VAL:HB	1:A:690:CYS:HB2	1.77	0.65
1:A:501:THR:HG21	1:A:510:PHE:HD1	1.62	0.65
1:A:815:PHE:HB2	1:A:831:MET:CE	2.28	0.64
1:B:276:VAL:HB	1:B:319:VAL:CG1	2.27	0.64
1:B:276:VAL:HB	1:B:319:VAL:HG11	1.78	0.64
1:B:532:THR:HG23	1:B:535:MET:H	1.62	0.64
1:A:126:LYS:HE2	1:A:166:ARG:NH2	2.12	0.64
1:B:258:GLU:HB3	1:B:261:ILE:HD12	1.79	0.64
1:A:72:HIS:CE1	1:A:773:ARG:HD2	2.32	0.64
1:A:193:MET:O	1:A:197:THR:HG23	1.97	0.64
1:A:200:VAL:HG21	1:A:245:ILE:HD12	1.79	0.64
1:A:21:THR:HG22	1:A:24:ASN:CG	2.18	0.64
1:B:166:ARG:NH2	1:B:373:ASP:OD2	2.30	0.64
1:B:41:ILE:HD12	1:B:46:PRO:HD3	1.78	0.64
1:B:5:GLN:O	1:B:9:VAL:HG23	1.97	0.64
1:A:535:MET:O	1:A:538:MET:HG2	1.96	0.64
1:A:183:LYS:CD	1:A:183:LYS:H	2.08	0.63
1:A:264:LYS:HA	1:A:264:LYS:HE3	1.80	0.63
1:A:731:ARG:NH1	1:A:865:GLN:HE21	1.96	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:PRO:HB3	1:A:261:ILE:HD13	1.81	0.63
1:B:324:GLU:CD	1:B:324:GLU:H	2.02	0.63
1:A:126:LYS:HE2	1:A:166:ARG:HH21	1.62	0.63
1:A:456:ARG:O	1:A:591:THR:HG23	1.99	0.63
1:A:50:PHE:HZ	1:A:83:VAL:HG13	1.62	0.63
1:B:283:ALA:HB3	1:B:284:PRO:CD	2.29	0.63
1:A:757:TRP:CH2	1:A:765:ARG:HD2	2.34	0.62
1:A:491:THR:HG22	1:A:563:ILE:HB	1.80	0.62
1:B:219:PRO:O	1:B:222:VAL:HG23	2.00	0.62
1:A:922:PRO:O	1:A:931:LEU:HD21	2.00	0.62
1:B:313:LEU:O	1:B:317:ARG:HG3	2.00	0.62
1:B:794:ARG:HD3	1:B:831:MET:CE	2.30	0.61
1:B:815:PHE:HB2	1:B:831:MET:HE3	1.81	0.61
1:B:45:VAL:HG11	1:B:86:TYR:CZ	2.35	0.61
1:B:45:VAL:HG11	1:B:86:TYR:CE2	2.35	0.61
1:B:36:LEU:HD23	1:B:73:ILE:HD13	1.83	0.61
1:A:916:LEU:HD23	1:A:944:GLY:HA3	1.82	0.61
1:B:936:LYS:O	1:B:940:GLU:HG3	2.00	0.60
1:A:815:PHE:HB2	1:A:831:MET:HE1	1.82	0.60
1:B:555:ARG:NH2	1:B:559:ARG:HH21	1.99	0.60
1:B:710:ILE:HD13	1:B:948:ILE:HD13	1.81	0.60
1:B:202:ASN:OD1	1:B:204:ASP:HB2	2.02	0.60
1:B:222:VAL:HB	1:B:223:PRO:HD3	1.82	0.60
1:B:774:GLN:C	1:B:776:ASN:N	2.54	0.60
1:A:45:VAL:HG11	1:A:86:TYR:OH	2.02	0.60
1:B:877:HIS:HE1	1:B:907:ALA:O	1.85	0.59
1:A:832:MET:O	1:A:834:VAL:N	2.35	0.59
1:A:69:ALA:O	1:A:73:ILE:HG13	2.03	0.59
1:B:774:GLN:C	1:B:776:ASN:H	2.05	0.59
1:B:494:VAL:O	1:B:496:HIS:HD2	1.86	0.59
1:B:538:MET:CE	1:B:542:ALA:HB3	2.33	0.58
1:A:102:ASP:OD2	1:A:105:ILE:HG13	2.03	0.58
1:A:501:THR:HG21	1:A:510:PHE:CD1	2.38	0.58
1:B:538:MET:HE3	1:B:542:ALA:HB3	1.86	0.58
1:A:538:MET:HE2	1:A:542:ALA:HB3	1.85	0.58
1:B:183:LYS:N	1:B:183:LYS:HD3	2.18	0.58
1:B:673:PHE:CZ	1:B:717:LEU:HD13	2.39	0.58
1:B:634:ALA:HB1	1:B:637:TYR:CZ	2.39	0.58
1:A:45:VAL:HG11	1:A:86:TYR:CE2	2.38	0.57
1:A:794:ARG:CD	1:A:831:MET:HE1	2.34	0.57
1:A:603:ASP:HA	1:A:623:ASN:HB2	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:ASP:HA	1:A:453:LYS:HE2	1.86	0.57
1:B:40:ILE:HG13	1:B:41:ILE:HG13	1.86	0.57
1:A:19:VAL:O	1:A:19:VAL:HG12	2.02	0.57
1:B:222:VAL:O	1:B:226:VAL:HG23	2.04	0.57
1:B:283:ALA:HB3	1:B:284:PRO:HD3	1.86	0.57
1:B:145:LYS:HE2	1:B:180:ASP:OD1	2.03	0.57
1:B:102:ASP:OD2	1:B:105:ILE:HG13	2.04	0.57
1:A:525:LYS:HE2	1:A:557:VAL:CG1	2.33	0.57
1:B:898:GLY:O	1:B:902:VAL:HG23	2.04	0.57
1:A:757:TRP:CZ2	1:A:765:ARG:HD2	2.40	0.57
1:B:262:LYS:HB3	1:B:296:ASN:ND2	2.20	0.57
1:A:21:THR:HG22	1:A:24:ASN:OD1	2.05	0.57
1:A:729:ASN:ND2	1:A:865:GLN:HG3	2.18	0.57
1:A:265:SER:O	1:A:269:ILE:HG13	2.04	0.57
1:A:731:ARG:NH1	1:A:865:GLN:NE2	2.54	0.56
1:B:671:MET:HG2	1:B:672:GLU:N	2.20	0.56
1:A:21:THR:HG23	1:A:23:ASP:N	2.17	0.56
1:A:372:ILE:HD11	1:A:410:ALA:HB1	1.87	0.56
1:B:535:MET:O	1:B:538:MET:HG2	2.05	0.56
1:B:45:VAL:O	1:B:47:GLU:N	2.38	0.56
1:B:643:THR:C	1:B:645:LEU:H	2.08	0.56
1:B:639:GLU:O	1:B:641:SER:N	2.39	0.56
1:A:850:LYS:O	1:A:854:GLU:HG3	2.06	0.56
1:B:463:PRO:HG2	1:B:466:CYS:HB3	1.87	0.56
1:B:90:LEU:O	1:B:94:ILE:HG13	2.06	0.55
1:B:613:GLU:OE1	1:B:618:ARG:HG3	2.06	0.55
1:A:794:ARG:HG2	1:A:831:MET:HE2	1.87	0.55
1:A:499:ASP:OD2	1:A:501:THR:HG23	2.06	0.55
1:A:276:VAL:HB	1:A:319:VAL:CG1	2.36	0.55
1:B:135:ALA:O	1:B:139:THR:HG22	2.07	0.55
1:B:195:LYS:O	1:B:198:GLU:HB2	2.06	0.55
1:A:671:MET:CG	1:A:672:GLU:N	2.68	0.55
1:B:262:LYS:HB3	1:B:296:ASN:HD22	1.71	0.55
1:B:372:ILE:O	1:B:375:ARG:NH1	2.37	0.55
1:B:884:ASP:HB3	1:B:887:ILE:HD12	1.89	0.55
1:B:53:LEU:O	1:B:57:ILE:HG13	2.07	0.54
1:A:422:ASP:HA	1:A:424:GLU:OE1	2.06	0.54
1:B:320:GLY:O	1:B:321:ASN:HB3	2.06	0.54
1:A:858:LYS:HE2	1:B:428:GLU:OE2	2.07	0.54
1:A:200:VAL:CG2	1:A:245:ILE:HD12	2.37	0.54
1:A:455:ALA:N	1:A:591:THR:OG1	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:LYS:HD3	1:B:185:VAL:HG11	1.89	0.54
1:B:223:PRO:HG3	1:B:256:GLU:HG2	1.88	0.54
1:A:969:ARG:NH1	1:A:969:ARG:HG3	2.19	0.54
1:B:67:MET:HE1	1:B:94:ILE:HG23	1.89	0.54
1:A:881:LEU:HD13	1:A:907:ALA:CB	2.36	0.54
1:A:532:THR:HG22	1:A:535:MET:CG	2.38	0.54
1:A:881:LEU:CD1	1:A:907:ALA:HA	2.37	0.54
1:A:916:LEU:CD2	1:A:944:GLY:HA3	2.37	0.54
1:B:747:LEU:HB3	1:B:894:ARG:HB2	1.90	0.54
1:B:538:MET:HB2	1:B:539:PRO:HD2	1.90	0.54
1:B:129:LEU:HB3	1:B:130:PRO:HD3	1.90	0.54
1:A:774:GLN:C	1:A:776:ASN:H	2.11	0.53
1:B:20:ALA:HB3	1:B:65:ASN:ND2	2.23	0.53
1:B:764:ASP:OD1	1:B:766:GLU:HB2	2.09	0.53
1:B:273:CYS:C	1:B:275:LEU:H	2.12	0.53
1:A:486:GLN:OE1	1:A:490:ARG:HD2	2.08	0.53
1:A:674:GLN:HB2	1:A:681:PRO:HB3	1.90	0.53
1:B:258:GLU:O	1:B:262:LYS:HG3	2.08	0.53
1:B:200:VAL:HG12	1:B:202:ASN:H	1.74	0.53
1:A:583:ASN:ND2	2:A:2976:SO4:O4	2.42	0.53
1:A:538:MET:CE	1:A:542:ALA:HB3	2.38	0.52
1:B:916:LEU:HD23	1:B:944:GLY:HA3	1.91	0.52
1:B:69:ALA:O	1:B:73:ILE:HG13	2.09	0.52
1:A:340:THR:O	1:A:344:VAL:HG22	2.10	0.52
1:B:386:ILE:HG22	1:B:390:MET:HG2	1.92	0.52
1:B:695:ARG:HB3	1:B:959:THR:HA	1.92	0.52
1:A:532:THR:CG2	1:A:535:MET:HG3	2.40	0.52
1:A:335:GLY:HA3	1:A:373:ASP:OD1	2.09	0.52
1:B:183:LYS:H	1:B:183:LYS:CD	2.22	0.52
1:A:50:PHE:CZ	1:A:83:VAL:HG13	2.45	0.52
1:B:815:PHE:HB2	1:B:831:MET:HE2	1.91	0.52
1:A:166:ARG:NH2	1:A:373:ASP:OD2	2.32	0.52
1:B:719:PRO:HG2	1:B:806:LYS:HD3	1.92	0.51
1:A:193:MET:HE2	1:A:216:ILE:HD12	1.91	0.51
1:B:734:TYR:CE2	1:B:736:LYS:HD2	2.46	0.51
1:B:169:GLU:O	1:B:172:PRO:HG2	2.10	0.51
1:A:773:ARG:HG2	1:A:773:ARG:HH11	1.75	0.51
1:B:123:VAL:HG13	1:B:370:ASP:OD2	2.10	0.51
1:A:318:ARG:NE	1:A:423:GLU:HG3	2.25	0.51
1:B:247:VAL:HG21	1:B:285:PHE:CD1	2.45	0.51
1:A:317:ARG:HG2	1:A:322:VAL:HG21	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:773:ARG:HG2	1:B:846:GLU:CD	2.31	0.51
1:A:639:GLU:O	1:A:641:SER:N	2.44	0.51
1:A:773:ARG:O	1:A:775:ILE:HG13	2.11	0.51
1:B:267:VAL:CG2	1:B:308:VAL:HG11	2.40	0.51
1:B:750:THR:OG1	1:B:753:GLU:HG3	2.10	0.51
1:B:532:THR:HG23	1:B:535:MET:HG3	1.93	0.51
1:A:802:ARG:HB3	1:A:859:GLU:HG3	1.93	0.51
1:B:653:GLY:O	1:B:915:HIS:HE1	1.94	0.50
1:A:212:LEU:CD2	1:A:249:LEU:HD22	2.42	0.50
1:A:494:VAL:O	1:A:496:HIS:HD2	1.95	0.50
1:A:543:LEU:O	1:A:548:LYS:HE3	2.12	0.50
1:A:435:PHE:CD1	1:A:480:VAL:HG13	2.46	0.50
1:A:177:THR:HG22	1:A:189:ALA:HB2	1.94	0.50
1:A:816:LEU:HD23	1:A:830:PRO:HA	1.92	0.50
1:A:494:VAL:HG13	1:A:552:ALA:HB1	1.94	0.50
1:A:763:GLU:OE1	1:A:768:MET:CE	2.60	0.50
1:B:666:VAL:HB	1:B:690:CYS:HB2	1.94	0.50
1:A:532:THR:CG2	1:A:535:MET:H	2.22	0.49
1:B:814:SER:HA	1:B:836:ASN:OD1	2.12	0.49
1:B:113:LEU:O	1:B:117:VAL:HG23	2.11	0.49
1:B:508:LEU:HB2	1:B:536:ILE:HG22	1.94	0.49
1:A:714:THR:HG21	1:A:734:TYR:CE1	2.48	0.49
1:B:757:TRP:CZ2	1:B:765:ARG:HD2	2.47	0.49
1:A:197:THR:HG22	1:A:245:ILE:CD1	2.41	0.49
1:A:372:ILE:CD1	1:A:410:ALA:HB1	2.42	0.49
1:A:77:SER:HA	1:A:738:HIS:CE1	2.47	0.49
1:B:731:ARG:N	1:B:915:HIS:HD2	2.01	0.49
1:B:223:PRO:HB3	1:B:261:ILE:CD1	2.43	0.49
1:B:420:PHE:HB3	1:B:619:LYS:HB3	1.94	0.49
1:B:603:ASP:HA	1:B:623:ASN:HB2	1.95	0.49
1:B:58:LYS:HE3	1:B:93:ALA:HB2	1.93	0.49
1:A:662:GLN:H	1:A:662:GLN:NE2	2.11	0.49
1:B:805:PHE:O	1:B:806:LYS:HB2	2.13	0.49
1:A:803:ARG:HG2	1:A:838:TRP:CZ3	2.48	0.49
1:B:869:LEU:HD23	1:B:911:TRP:CZ2	2.48	0.49
1:B:785:LYS:HD3	1:B:787:PHE:CZ	2.47	0.48
1:B:324:GLU:O	1:B:325:ASP:HB2	2.12	0.48
1:A:832:MET:C	1:A:834:VAL:H	2.17	0.48
1:B:440:GLY:O	1:B:441:ALA:HB3	2.13	0.48
1:B:532:THR:HG22	1:B:535:MET:SD	2.53	0.48
1:A:400:LYS:NZ	1:A:923:THR:O	2.45	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:PHE:CD1	1:A:394:LEU:HG	2.48	0.48
1:A:129:LEU:HB3	1:A:130:PRO:HD3	1.95	0.48
1:B:969:ARG:HH11	1:B:969:ARG:HG2	1.78	0.48
1:B:387:THR:HB	1:B:388:PRO:CD	2.44	0.48
1:A:212:LEU:HD13	1:A:245:ILE:HG22	1.96	0.48
1:A:195:LYS:O	1:A:198:GLU:HB2	2.14	0.48
1:A:752:SER:O	1:A:756:GLN:HG3	2.12	0.48
1:A:499:ASP:OD2	1:A:510:PHE:HE1	1.96	0.48
1:A:424:GLU:HG2	1:A:424:GLU:O	2.12	0.48
1:B:35:PHE:HB2	1:B:675:TYR:CZ	2.49	0.48
1:B:7:ILE:O	1:B:11:GLU:HG2	2.14	0.48
1:A:313:LEU:HD21	1:A:317:ARG:NH2	2.28	0.48
1:B:956:LYS:O	1:B:957:ASN:HB2	2.14	0.48
1:B:634:ALA:O	1:B:637:TYR:CD2	2.66	0.48
1:B:25:ARG:HD3	1:B:65:ASN:HA	1.96	0.48
1:A:393:PHE:O	1:A:394:LEU:HD23	2.13	0.48
1:B:728:GLU:O	1:B:729:ASN:HB2	2.14	0.48
1:A:737:GLN:HG3	1:A:738:HIS:N	2.28	0.47
1:A:773:ARG:C	1:A:775:ILE:H	2.17	0.47
1:B:136:ILE:HB	1:B:148:ILE:HG21	1.96	0.47
1:A:159:ALA:HB1	1:A:162:GLN:HB2	1.97	0.47
1:A:710:ILE:CD1	1:A:948:ILE:HD13	2.44	0.47
1:A:440:GLY:O	1:A:441:ALA:HB3	2.14	0.47
1:A:447:LYS:O	1:A:616:LYS:NZ	2.46	0.47
1:B:501:THR:HG21	1:B:510:PHE:CD1	2.49	0.47
1:B:754:TYR:HB2	1:B:893:ILE:HD11	1.97	0.47
1:B:89:GLN:NE2	1:B:359:ILE:HD13	2.30	0.47
1:B:928:ARG:HB2	1:B:928:ARG:NH1	2.30	0.47
1:B:262:LYS:HE3	1:B:296:ASN:CG	2.35	0.47
1:A:372:ILE:HD11	1:A:410:ALA:CB	2.44	0.47
1:A:283:ALA:HB3	1:A:284:PRO:CD	2.45	0.47
1:A:710:ILE:HG12	1:A:948:ILE:HD13	1.97	0.47
1:B:267:VAL:HG22	1:B:308:VAL:HG11	1.95	0.47
1:B:684:THR:CG2	1:B:969:ARG:HE	2.27	0.47
1:A:61:LYS:HD3	1:A:62:THR:HG23	1.96	0.47
1:A:916:LEU:HD23	1:A:944:GLY:CA	2.46	0.46
1:A:727:HIS:ND1	1:A:728:GLU:O	2.46	0.46
1:A:728:GLU:O	1:A:729:ASN:HB2	2.15	0.46
1:B:28:ILE:O	1:B:32:VAL:HG23	2.15	0.46
1:A:304:GLU:HG3	1:A:305:ALA:N	2.30	0.46
1:A:263:ARG:NH1	1:A:308:VAL:HG21	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:ILE:HG23	1:A:386:ILE:CG2	2.46	0.46
1:A:263:ARG:CZ	1:A:304:GLU:OE1	2.64	0.46
1:A:471:LEU:O	1:A:475:ILE:HG13	2.15	0.46
1:A:39:ASN:O	1:A:702:ASN:HB3	2.15	0.46
1:B:680:LYS:HB2	1:B:681:PRO:HD2	1.98	0.46
1:B:193:MET:O	1:B:197:THR:HG23	2.15	0.46
1:B:881:LEU:HD22	1:B:907:ALA:N	2.30	0.46
1:A:393:PHE:CE1	1:A:394:LEU:HG	2.50	0.46
1:B:939:LYS:HE2	1:B:957:ASN:O	2.16	0.46
1:B:754:TYR:CZ	1:B:758:ARG:HD2	2.50	0.46
1:B:674:GLN:HB2	1:B:681:PRO:HA	1.97	0.46
1:B:39:ASN:O	1:B:702:ASN:HB3	2.15	0.46
1:A:653:GLY:O	1:A:915:HIS:HE1	2.00	0.45
1:A:802:ARG:HG2	1:A:803:ARG:N	2.31	0.45
1:A:763:GLU:OE1	1:A:768:MET:HE1	2.16	0.45
1:B:391:THR:HG21	1:B:924:ASN:OD1	2.16	0.45
1:B:642:ASN:O	1:B:645:LEU:HB3	2.16	0.45
1:B:674:GLN:HB2	1:B:681:PRO:HB3	1.97	0.45
1:B:404:ASP:OD1	1:B:407:ARG:NH1	2.49	0.45
1:B:50:PHE:HZ	1:B:83:VAL:CG1	2.21	0.45
1:A:245:ILE:HG22	1:A:245:ILE:O	2.16	0.45
1:B:638:GLU:HG3	1:B:639:GLU:N	2.31	0.45
1:B:125:ILE:HG23	1:B:126:LYS:N	2.31	0.45
1:B:425:ASP:OD1	1:B:426:GLU:HG2	2.16	0.45
1:A:877:HIS:HE1	1:A:907:ALA:O	2.00	0.45
1:A:814:SER:HA	1:A:836:ASN:OD1	2.17	0.45
1:A:634:ALA:C	1:A:636:ALA:H	2.20	0.45
1:B:730:CYS:HA	1:B:915:HIS:CD2	2.52	0.45
1:A:42:GLU:OE1	1:A:950:HIS:HE1	1.99	0.45
1:B:67:MET:HE1	1:B:109:ALA:HA	1.94	0.45
1:A:197:THR:HG22	1:A:245:ILE:HD13	1.97	0.45
1:B:223:PRO:HB3	1:B:261:ILE:HD11	1.99	0.45
1:A:794:ARG:HB3	1:A:815:PHE:HB3	1.98	0.45
1:A:654:TYR:OH	2:A:2978:SO4:O2	2.33	0.45
1:A:521:ALA:HB2	1:B:654:TYR:CE2	2.52	0.45
1:B:301:ALA:HB3	2:B:2974:SO4:O3	2.17	0.45
1:B:769:ASP:HB2	1:B:774:GLN:HE22	1.64	0.44
1:A:815:PHE:HB2	1:A:831:MET:HE3	1.96	0.44
1:B:263:ARG:O	1:B:267:VAL:HG23	2.17	0.44
1:B:2:ASP:OD2	1:B:703:GLY:HA3	2.17	0.44
1:A:729:ASN:HD21	1:A:863:SER:HB2	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:652:PRO:HD2	1:B:942:GLU:HB2	1.99	0.44
1:A:430:LEU:HD13	1:A:563:ILE:CG1	2.47	0.44
1:A:858:LYS:HG3	1:B:454:ARG:HD3	1.99	0.44
1:B:390:MET:HE3	1:B:390:MET:HB3	1.84	0.44
1:B:393:PHE:CD1	1:B:394:LEU:HG	2.52	0.44
1:B:301:ALA:N	2:B:2974:SO4:O1	2.38	0.44
1:A:432:ASN:HB2	1:A:451:ARG:HG3	1.99	0.44
1:B:816:LEU:HD23	1:B:830:PRO:HA	1.99	0.44
1:B:671:MET:CG	1:B:672:GLU:N	2.81	0.44
1:B:555:ARG:NH2	1:B:559:ARG:NH2	2.64	0.44
1:B:458:TYR:CD1	1:B:608:TYR:HB2	2.52	0.44
1:A:335:GLY:O	1:A:369:ALA:HB1	2.17	0.44
1:A:596:SER:O	1:A:639:GLU:OE1	2.35	0.44
1:A:391:THR:HA	1:A:394:LEU:O	2.18	0.44
1:A:871:ARG:CG	1:A:871:ARG:HH11	2.31	0.44
1:A:884:ASP:HA	1:A:885:PRO:HD3	1.91	0.44
1:A:732:ILE:HG12	1:A:916:LEU:HB2	1.99	0.44
1:A:799:ILE:HG23	1:A:811:TYR:HB3	2.00	0.44
1:B:112:THR:O	1:B:116:ILE:HG13	2.17	0.44
1:A:126:LYS:CE	1:A:166:ARG:NH2	2.80	0.44
1:B:167:MET:N	1:B:168:PRO:HD2	2.33	0.44
1:B:280:GLN:OE1	1:B:332:SER:HB3	2.18	0.43
1:B:921:GLU:CD	1:B:949:THR:HA	2.39	0.43
1:B:297:PHE:CZ	1:B:310:LEU:HD13	2.53	0.43
1:A:407:ARG:O	1:A:411:VAL:HG23	2.18	0.43
1:A:372:ILE:HD11	1:A:410:ALA:C	2.39	0.43
1:B:774:GLN:O	1:B:775:ILE:C	2.55	0.43
1:B:425:ASP:OD1	1:B:426:GLU:N	2.49	0.43
1:A:705:GLY:HA3	1:A:965:VAL:HG11	2.00	0.43
1:B:708:THR:O	1:B:712:VAL:HG23	2.17	0.43
1:A:21:THR:CG2	1:A:24:ASN:H	2.31	0.43
1:A:662:GLN:N	1:A:662:GLN:NE2	2.67	0.43
1:B:453:LYS:HB3	1:B:456:ARG:CG	2.48	0.43
1:B:83:VAL:CG1	1:B:83:VAL:O	2.66	0.43
1:B:571:ASN:O	1:B:572:HIS:HB2	2.18	0.43
1:A:562:ASP:O	1:A:590:ILE:HG23	2.19	0.43
1:B:970:MET:HB3	1:B:970:MET:HE2	1.74	0.43
1:A:737:GLN:HE21	1:A:737:GLN:HB2	1.54	0.43
1:B:451:ARG:HD3	1:B:453:LYS:NZ	2.33	0.43
1:B:207:ARG:HG2	1:B:207:ARG:HH11	1.82	0.43
1:B:123:VAL:HG12	1:B:367:ILE:HG23	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:LYS:HE2	1:B:184:GLU:OE2	2.18	0.43
1:B:278:ASP:HB3	1:B:281:VAL:HG23	2.00	0.43
1:B:634:ALA:C	1:B:636:ALA:H	2.21	0.42
1:B:317:ARG:HA	1:B:322:VAL:HG22	2.01	0.42
1:A:370:ASP:OD2	1:A:374:GLU:OE1	2.37	0.42
1:B:239:THR:HB	1:B:240:PRO:HD2	2.02	0.42
1:B:166:ARG:HD3	1:B:166:ARG:HA	1.69	0.42
1:B:875:GLU:O	1:B:879:SER:HB2	2.19	0.42
1:A:713:LEU:HD21	1:A:946:ILE:HD13	2.01	0.42
1:B:374:GLU:O	1:B:375:ARG:HB2	2.19	0.42
1:B:508:LEU:HB2	1:B:536:ILE:CG2	2.50	0.42
1:B:499:ASP:OD1	1:B:501:THR:HG23	2.20	0.42
1:A:869:LEU:HD23	1:A:911:TRP:CZ2	2.54	0.42
1:A:383:PHE:HA	1:A:403:LEU:HD21	2.02	0.42
1:A:768:MET:O	1:A:769:ASP:HB2	2.20	0.42
1:A:769:ASP:OD1	1:A:845:VAL:HG21	2.19	0.42
1:B:420:PHE:CB	1:B:619:LYS:HB3	2.49	0.42
1:A:263:ARG:HH21	1:B:781:GLU:HA	1.84	0.42
1:B:804:LYS:HE3	1:B:806:LYS:O	2.19	0.42
1:A:516:VAL:HG12	1:A:559:ARG:HG2	2.01	0.42
1:B:359:ILE:HG23	1:B:360:VAL:N	2.35	0.42
1:B:239:THR:HB	1:B:240:PRO:CD	2.50	0.42
1:B:611:ASN:ND2	1:B:612:TYR:H	2.17	0.42
1:A:740:PHE:HA	1:A:905:VAL:HG21	2.01	0.42
1:B:301:ALA:O	1:B:302:ASP:C	2.57	0.42
1:A:799:ILE:CG2	1:A:811:TYR:HB3	2.49	0.42
1:B:77:SER:HA	1:B:738:HIS:CE1	2.55	0.42
1:B:16:LYS:HD2	1:B:677:GLY:HA3	2.01	0.42
1:B:423:GLU:HG2	1:B:451:ARG:NH2	2.34	0.42
1:B:780:ALA:O	1:B:783:MET:SD	2.78	0.42
1:A:797:ALA:HB3	1:A:814:SER:O	2.20	0.42
1:B:446:ASN:O	1:B:616:LYS:NZ	2.44	0.42
1:A:219:PRO:O	1:A:222:VAL:HG23	2.19	0.42
1:B:186:LYS:HE3	1:B:186:LYS:HB2	1.87	0.42
1:B:313:LEU:HD21	1:B:317:ARG:HH21	1.85	0.41
1:B:121:ASN:OD1	1:B:123:VAL:HB	2.18	0.41
1:A:516:VAL:HG23	1:A:517:GLY:N	2.35	0.41
1:A:773:ARG:HG2	1:A:773:ARG:NH1	2.34	0.41
1:A:278:ASP:HB3	1:A:281:VAL:HG23	2.01	0.41
1:A:970:MET:HG2	1:A:971:THR:N	2.29	0.41
1:B:422:ASP:O	1:B:424:GLU:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:916:LEU:CD2	1:B:944:GLY:HA3	2.50	0.41
1:A:657:GLY:N	2:A:2978:SO4:O1	2.50	0.41
1:A:897:SER:O	1:A:901:LYS:HG3	2.21	0.41
1:B:358:LYS:O	1:B:362:GLU:HG3	2.19	0.41
1:A:387:THR:N	1:A:388:PRO:HD2	2.35	0.41
1:B:290:LEU:N	1:B:291:PRO:HD2	2.35	0.41
1:A:425:ASP:OD1	1:A:427:GLY:O	2.38	0.41
1:B:697:ALA:HB2	1:B:959:THR:OG1	2.21	0.41
1:B:29:ALA:HB1	1:B:69:ALA:HA	2.03	0.41
1:B:797:ALA:HB3	1:B:814:SER:OG	2.20	0.41
1:B:501:THR:HG21	1:B:510:PHE:CE1	2.55	0.41
1:A:14:PHE:CZ	1:A:52:GLU:HB3	2.56	0.41
1:B:491:THR:HG22	1:B:563:ILE:HB	2.01	0.41
1:B:413:ASN:HD22	1:B:413:ASN:N	2.17	0.41
1:B:652:PRO:HB3	1:B:915:HIS:HA	2.03	0.41
1:B:773:ARG:HG3	1:B:773:ARG:O	2.21	0.41
1:A:364:ILE:HD13	1:A:390:MET:HG2	2.01	0.41
1:B:572:HIS:O	1:B:573:LEU:HD12	2.20	0.41
1:A:971:THR:O	1:A:971:THR:HG23	2.18	0.41
1:A:947:ILE:HD13	1:A:954:PHE:CE2	2.55	0.41
1:A:454:ARG:O	1:A:455:ALA:HB3	2.21	0.41
1:B:238:VAL:HG21	1:B:272:MET:O	2.21	0.41
1:B:14:PHE:CZ	1:B:52:GLU:HB3	2.54	0.41
1:B:608:TYR:CD1	1:B:621:LYS:HA	2.56	0.41
1:B:716:GLU:HB2	1:B:770:ARG:NH2	2.36	0.41
1:A:829:VAL:HG13	1:A:830:PRO:HD2	2.02	0.41
1:A:328:ILE:HG23	1:A:329:PRO:HD2	2.01	0.41
1:A:214:GLN:HA	1:A:214:GLN:OE1	2.20	0.41
1:A:21:THR:N	1:A:24:ASN:OD1	2.43	0.41
1:B:532:THR:CG2	1:B:535:MET:CG	2.97	0.41
1:A:190:THR:O	1:A:193:MET:HB3	2.21	0.41
1:B:643:THR:C	1:B:645:LEU:N	2.74	0.41
1:A:446:ASN:O	1:A:616:LYS:NZ	2.48	0.41
1:A:449:GLN:N	1:A:449:GLN:CD	2.74	0.41
1:B:569:PRO:HB2	1:B:581:LEU:HD21	2.03	0.41
1:A:881:LEU:HD13	1:A:907:ALA:HB2	2.03	0.40
1:A:193:MET:CE	1:A:216:ILE:HD12	2.51	0.40
1:A:710:ILE:HD13	1:A:948:ILE:HD13	2.03	0.40
1:A:939:LYS:HE3	1:A:939:LYS:HB2	1.77	0.40
1:A:803:ARG:NH2	1:A:838:TRP:CD1	2.89	0.40
1:B:83:VAL:O	1:B:83:VAL:HG12	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:568:GLU:N	1:B:569:PRO:CD	2.85	0.40
1:B:60:LYS:H	1:B:60:LYS:HG3	1.76	0.40
1:B:300:ILE:HG21	1:B:305:ALA:HB3	2.03	0.40
1:B:811:TYR:CZ	1:B:852:VAL:HG13	2.56	0.40
1:A:296:ASN:O	1:A:300:ILE:HG13	2.21	0.40
1:B:887:ILE:O	1:B:891:SER:HB2	2.22	0.40
1:B:302:ASP:O	1:B:306:ARG:HG3	2.21	0.40
1:B:61:LYS:HD2	1:B:62:THR:HG23	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	971/986 (98%)	926 (95%)	41 (4%)	4 (0%)	39	69
1	B	971/986 (98%)	907 (93%)	59 (6%)	5 (0%)	34	63
All	All	1942/1972 (98%)	1833 (94%)	100 (5%)	9 (0%)	34	63

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	640	LEU
1	A	833	SER
1	B	640	LEU
1	B	775	ILE
1	A	775	ILE
1	B	20	ALA
1	B	284	PRO
1	A	845	VAL
1	B	283	ALA

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	831/843 (99%)	802 (96%)	29 (4%)	43	74
1	B	831/843 (99%)	807 (97%)	24 (3%)	50	80
All	All	1662/1686 (99%)	1609 (97%)	53 (3%)	46	77

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	39	ASN
1	A	62	THR
1	A	104	GLU
1	A	183	LYS
1	A	198	GLU
1	A	211	SER
1	A	263	ARG
1	A	264	LYS
1	A	304	GLU
1	A	316	LEU
1	A	338	SER
1	A	342	GLN
1	A	351	GLU
1	A	432	ASN
1	A	433	CYS
1	A	449	GLN
1	A	451	ARG
1	A	493	TYR
1	A	599	SER
1	A	618	ARG
1	A	737	GLN
1	A	773	ARG
1	A	804	LYS
1	A	827	ARG
1	A	858	LYS
1	A	867	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	922	PRO
1	A	953	GLU
1	B	23	ASP
1	B	166	ARG
1	B	180	ASP
1	B	183	LYS
1	B	206	GLU
1	B	330	GLU
1	B	342	GLN
1	B	358	LYS
1	B	431	CYS
1	B	432	ASN
1	B	493	TYR
1	B	525	LYS
1	B	532	THR
1	B	571	ASN
1	B	662	GLN
1	B	685	ASP
1	B	737	GLN
1	B	827	ARG
1	B	859	GLU
1	B	872	LYS
1	B	879	SER
1	B	958	LEU
1	B	969	ARG
1	B	970	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	97	ASN
1	A	271	ASN
1	A	321	ASN
1	A	413	ASN
1	A	432	ASN
1	A	496	HIS
1	A	577	ASN
1	A	604	ASN
1	A	611	ASN
1	A	662	GLN
1	A	711	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	729	ASN
1	A	737	GLN
1	A	756	GLN
1	A	848	HIS
1	A	865	GLN
1	A	877	HIS
1	A	915	HIS
1	B	24	ASN
1	B	76	GLN
1	B	89	GLN
1	B	97	ASN
1	B	296	ASN
1	B	321	ASN
1	B	342	GLN
1	B	413	ASN
1	B	432	ASN
1	B	449	GLN
1	B	496	HIS
1	B	604	ASN
1	B	611	ASN
1	B	642	ASN
1	B	662	GLN
1	B	674	GLN
1	B	711	ASN
1	B	774	GLN
1	B	784	ASN
1	B	848	HIS
1	B	877	HIS
1	B	915	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

11 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	2973	-	4,4,4	3.22	2 (50%)	6,6,6	0.51	0
2	SO4	A	2974	-	4,4,4	3.24	2 (50%)	6,6,6	0.49	0
2	SO4	A	2975	-	4,4,4	3.15	2 (50%)	6,6,6	0.50	0
2	SO4	A	2976	-	4,4,4	3.21	2 (50%)	6,6,6	0.49	0
2	SO4	A	2977	-	4,4,4	3.18	2 (50%)	6,6,6	0.51	0
2	SO4	A	2978	-	4,4,4	3.10	2 (50%)	6,6,6	0.50	0
2	SO4	B	2973	-	4,4,4	3.33	2 (50%)	6,6,6	0.51	0
2	SO4	B	2974	-	4,4,4	3.16	2 (50%)	6,6,6	3.20	3 (50%)
2	SO4	B	2975	-	4,4,4	3.24	2 (50%)	6,6,6	3.20	4 (66%)
2	SO4	B	2976	-	4,4,4	3.21	2 (50%)	6,6,6	0.51	0
2	SO4	B	2977	-	4,4,4	3.20	2 (50%)	6,6,6	0.51	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	2973	-	-	0/0/0/0	0/0/0/0
2	SO4	A	2974	-	-	0/0/0/0	0/0/0/0
2	SO4	A	2975	-	-	0/0/0/0	0/0/0/0
2	SO4	A	2976	-	-	0/0/0/0	0/0/0/0
2	SO4	A	2977	-	-	0/0/0/0	0/0/0/0
2	SO4	A	2978	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2973	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2974	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2975	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2976	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2977	-	-	0/0/0/0	0/0/0/0

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2973	SO4	O2-S	-4.78	1.30	1.47
2	B	2973	SO4	O2-S	-4.73	1.31	1.47
2	B	2975	SO4	O2-S	-4.71	1.31	1.47
2	A	2977	SO4	O2-S	-4.71	1.31	1.47
2	B	2977	SO4	O2-S	-4.55	1.31	1.47
2	A	2976	SO4	O2-S	-4.51	1.31	1.47
2	A	2974	SO4	O2-S	-4.48	1.31	1.47
2	B	2976	SO4	O2-S	-4.45	1.32	1.47
2	B	2974	SO4	O2-S	-4.42	1.32	1.47
2	A	2978	SO4	O2-S	-4.38	1.32	1.47
2	A	2975	SO4	O2-S	-4.29	1.32	1.47
2	A	2977	SO4	O1-S	4.13	1.61	1.47
2	A	2973	SO4	O1-S	4.24	1.61	1.47
2	B	2975	SO4	O1-S	4.29	1.61	1.47
2	A	2978	SO4	O1-S	4.35	1.62	1.47
2	B	2974	SO4	O1-S	4.38	1.62	1.47
2	B	2977	SO4	O1-S	4.40	1.62	1.47
2	A	2976	SO4	O1-S	4.48	1.62	1.47
2	B	2973	SO4	O1-S	4.49	1.62	1.47
2	B	2976	SO4	O1-S	4.51	1.62	1.47
2	A	2975	SO4	O1-S	4.54	1.62	1.47
2	A	2974	SO4	O1-S	4.61	1.62	1.47

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2974	SO4	O4-S-O3	-5.93	84.85	108.98
2	B	2975	SO4	O4-S-O3	-5.90	85.00	108.98
2	B	2974	SO4	O3-S-O1	-3.44	78.21	110.19
2	B	2975	SO4	O3-S-O1	-3.36	78.90	110.19
2	B	2975	SO4	O3-S-O2	-2.03	91.28	110.19
2	B	2974	SO4	O2-S-O1	2.95	118.84	109.50
2	B	2975	SO4	O2-S-O1	3.04	119.13	109.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2976	SO4	1	0
2	A	2978	SO4	2	0
2	B	2974	SO4	2	0
2	B	2977	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	973/986 (98%)	-0.06	30 (3%)	52 52	20, 41, 70, 120	0
1	B	973/986 (98%)	0.13	51 (5%)	31 30	24, 49, 79, 114	0
All	All	1946/1972 (98%)	0.04	81 (4%)	40 39	20, 44, 77, 120	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	640	LEU	11.4
1	A	778	ASN	9.4
1	B	642	ASN	7.4
1	B	641	SER	7.4
1	A	776	ASN	7.1
1	B	637	TYR	6.7
1	B	643	THR	6.6
1	B	639	GLU	6.5
1	A	777	GLU	6.3
1	B	775	ILE	6.1
1	B	426	GLU	5.7
1	B	779	ASP	5.7
1	B	424	GLU	5.6
1	B	778	ASN	5.6
1	B	774	GLN	5.5
1	A	423	GLU	4.9
1	A	779	ASP	4.7
1	B	780	ALA	4.7
1	A	425	ASP	4.4
1	B	416	VAL	4.2
1	A	833	SER	4.0
1	B	330	GLU	4.0
1	A	426	GLU	3.9
1	B	423	GLU	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	776	ASN	3.8
1	B	777	GLU	3.7
1	B	325	ASP	3.7
1	A	421	ASP	3.6
1	A	775	ILE	3.5
1	B	425	ASP	3.5
1	B	298	ALA	3.3
1	B	19	VAL	3.3
1	A	424	GLU	3.2
1	B	420	PHE	3.2
1	A	417	GLY	3.2
1	A	644	ASP	3.1
1	A	422	ASP	3.1
1	A	572	HIS	3.0
1	A	643	THR	3.0
1	B	638	GLU	2.9
1	A	427	GLY	2.9
1	B	257	ARG	2.9
1	B	103	LYS	2.9
1	B	422	ASP	2.8
1	B	101	LYS	2.8
1	B	324	GLU	2.8
1	B	447	LYS	2.8
1	B	572	HIS	2.8
1	B	61	LYS	2.7
1	A	257	ARG	2.7
1	A	641	SER	2.7
1	A	419	ASN	2.6
1	B	782	ALA	2.6
1	B	419	ASN	2.6
1	A	972	PRO	2.6
1	B	140	ASN	2.5
1	B	644	ASP	2.5
1	B	773	ARG	2.5
1	B	4	GLN	2.5
1	A	352	THR	2.5
1	B	1	SER	2.5
1	B	181	THR	2.4
1	B	397	LYS	2.3
1	B	331	LEU	2.3
1	A	642	ASN	2.3
1	B	2	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	231	ALA	2.3
1	B	323	GLY	2.3
1	A	659	LYS	2.2
1	B	504	ASP	2.2
1	B	333	HIS	2.2
1	A	69	ALA	2.2
1	A	23	ASP	2.2
1	B	364	ILE	2.1
1	A	179	TRP	2.1
1	B	634	ALA	2.1
1	A	825	SER	2.1
1	B	421	ASP	2.1
1	A	971	THR	2.0
1	A	781	GLU	2.0
1	B	957	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	B	2974	5/5	0.89	0.39	5.80	80,82,82,83	0
2	SO4	B	2975	5/5	0.93	0.29	3.64	85,85,85,86	0
2	SO4	A	2976	5/5	0.95	0.23	2.01	75,75,76,76	0
2	SO4	A	2978	5/5	0.82	0.34	1.40	94,94,95,96	0
2	SO4	B	2977	5/5	0.96	0.29	1.04	91,92,93,93	0
2	SO4	A	2973	5/5	0.97	0.19	-0.11	48,50,50,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	B	2973	5/5	0.96	0.19	-0.55	74,75,76,76	0
2	SO4	A	2977	5/5	0.98	0.11	-0.61	53,53,54,55	0
2	SO4	B	2976	5/5	0.98	0.09	-1.31	50,50,52,53	0
2	SO4	A	2975	5/5	0.89	0.26	-	93,93,94,94	0
2	SO4	A	2974	5/5	0.91	0.36	-	96,96,96,98	0

6.5 Other polymers [i](#)

There are no such residues in this entry.